

DIFFERENTIAL TRANSFER MATRIX SOLUTION OF GENERALIZED EIGENVALUE PROBLEMS

SINA KHORASANI

ABSTRACT. We report a new analytical method for solution of a wide class of second-order differential equations with eigenvalues replaced by arbitrary functions. Such classes of problems occur frequently in Quantum Mechanics and Optics. This approach is based on the extension of the previously reported differential transfer matrix method with modified basis functions. Applications of the method to boundary value and initial value problems, as well as several examples are illustrated.

1. INTRODUCTION

Analytical solution of differential equations provides insight to the behavior of solutions whenever they exist. Unfortunately, most practical physical problems are described by governing models which are normally solved by numerical techniques. Moreover, explicit solutions even to the simplest differential equations are rare. A wide class of physical problems are described by second-order differential equations, where the only known analytical method with explicit solution for this purpose is the approximate Wentzel–Kramers–Brillouin (WKB) method [1, 2]. An approximate method for solution of linear homogeneous differential equations with variable coefficients has been reported in [3], which is based on a transformation into a Volterra or Fredholm integral equation. Also, a matrix method has been reported in [4] which is used to transform the Schrödinger equation into a ShabatZakharov system of second order, and then the solution is obtained by perturbation technique. There are also a number of further existing analytical methods for solution of Ordinary Differential Equations which are categorized and reviewed by Polyanin and Zaitsev in [5].

Recently, we have introduced an analytical method which is capable of solving linear homogeneous Ordinary Differential Equations (ODEs) with variable coefficients [6]. The method is based on the definition of jump transfer matrices and taking the differential limit. The approach reduces the n th-order differential equation to a first order system of n linear differential equations. The full analytical solution is then found by the perturbation technique, which may be elegantly expressed in terms of matrix exponentiation of the integral of a Kernel matrix. The important feature of this method is that it deals with the evolution of independent solutions, rather than its derivatives. The exact mathematical nature of this method has also been rigorously established [6].

This method emerged as an extension of Differential Transfer Matrix Method (DTMM), which was originally proposed in the context of optics and quantum mechanics [7, 8, 9]. DTMM is based on the modification of the standard transfer matrix method in optics [10] and quantum mechanics [11], and employs exponential

basis functions. Through numerous examples, this method was shown to be simple, exact, and efficient, while reflecting the basic properties of the physical problem.

However, the initial formulation of DTMM had difficulty when dealing with singularities. Such singularities arise in the domain of optics and quantum mechanics at the turning points of wavefunctions, where the behavior switches between oscillatory and decaying forms [2]. As a result, basic DTMM results suffer from numerical error when approaching physical singularities. To overcome this difficulty, the solution may be expressed by using Airy functions [2]. Further applications and extensions of DTMM have been reported by Mehrany et. al., which include employment of WKB basis [12, 13] for improvement of numerical accuracy, and numerical implementation of the method using Airy functions [14] for dealing with singularities. Also, the original DTMM has been used in [15] with no essential change as reported in the main formulation [6].

In this paper, we report a general formulation of DTMM for eigenvalue problems having second-order ODEs. The generalization is done by replacing the eigenvalue with an arbitrary function, which we here refer to as the eigenvalue function. We show that DTMM is still capable of delivering the analytical solution provided that proper basis functions are used. We also establish the mathematical validity of this method by presenting the fundamental theorem of DTMM. The major improvement of this work in contrast to the original formulation [6] is two-fold. Firstly, the solution to the extended eigenvalue problem evolves ‘naturally’ out of the relevant basis functions rather than exponentials. Secondly, envelope functions undergo minimal variations because most of the solution is encompassed in the extended bases. As a result, we may obtain a simple approximate solution for problems with slowly varying eigenvalue functions.

2. FORMULATION

Suppose that a linear homogeneous ordinary differential equation (ODE) is given as

$$\mathbb{H}_k f(x; k) = 0 \quad (1)$$

where \mathbb{H}_k is a second-order linear operator with eigenvalue k which involves partial derivatives only with respect to x , and $f(x; k)$ being its eigenfunction. It is the purpose of this formulation to find solutions of (1) when the eigenvalue k is replaced by an eigenvalue function such as $k(x)$. Hence, the extended problem reads

$$\mathbb{L}_{k(x)} f[x; k(x)] = 0 \quad (2)$$

Here, the new operator $\mathbb{L}_{k(x)}$ is obtained from \mathbb{H}_k by replacing the eigenvalue k with an eigenvalue function $k(x)$, and $\partial/\partial x$ with d/dx . In general, (1) admits a general solution having the form

$$f(x; k) = aA(x; k) + bB(x; k) \quad (3)$$

in which a and b are constants determined by initial or boundary conditions, and $A(x; k)$ and $B(x; k)$ are linearly independent solutions with non-vanishing Wronskian determinant, i.e.

$$W(x; k) = \begin{vmatrix} A(x; k) & B(x; k) \\ A_x(x; k) & B_x(x; k) \end{vmatrix} \neq 0 \quad (4)$$

Clearly, $A_x(x; k) = \partial A(x; k)/\partial x$ and $B_x(x; k) = \partial B(x; k)/\partial x$.

Now, we seek a solution to (2) having the extended form to (3) given by

$$f(x; k) = a(x) A[x; k(x)] + b(x) B[x; k(x)] \quad (5)$$

where $a(x)$ and $b(x)$ remain as unknown functions to be determined.

2.1. Transfer Matrix of Finite Jumps. In order to proceed with the formulation, we take a similar approach to the conventional Differential Transfer Matrix Method with exponential basis. For this reason, we first need to obtain the transfer matrix of finite jumps in the eigenvalue k . Suppose that the eigenvalue function is $k(x)$ defined as

$$k(x) = \begin{cases} k_1, & x > X \\ k_2, & x < X \end{cases} \quad (6)$$

with k_1 , k_2 , and X being constants. Solution to (1) is readily given by (3) as

$$\begin{aligned} f[x; k(x)] &= \begin{cases} f_1(x), & x < X \\ f_2(x), & x > X \end{cases} \\ &= \begin{cases} a_1 A(x; k_1) + b_1 B(x; k_1), & x < X \\ a_2 A(x; k_2) + b_2 B(x; k_2), & x > X \end{cases} \end{aligned} \quad (7)$$

Analyticity of $f[x; k(x)]$ across requires that

$$\begin{aligned} f_1(X) &= f_2(X) \\ f'_1(X) &= f'_2(X) \end{aligned} \quad (8)$$

We hence arrive in the system of equations

$$\begin{bmatrix} A(X; k_2) & B(X; k_2) \\ A_x(X; k_2) & B_x(X; k_2) \end{bmatrix} \begin{Bmatrix} a_2 \\ b_2 \end{Bmatrix} = \begin{bmatrix} A(X; k_1) & B(X; k_1) \\ A_x(X; k_1) & B_x(X; k_1) \end{bmatrix} \begin{Bmatrix} a_1 \\ b_1 \end{Bmatrix} \quad (9)$$

Since the Wronskian W is supposed to be non-zero by (4), then (9) can be solved to obtain

$$\begin{Bmatrix} a_2 \\ b_2 \end{Bmatrix} = \begin{bmatrix} A_2 & B_2 \\ A'_2 & B'_2 \end{bmatrix}^{-1} \begin{bmatrix} A_1 & B_1 \\ A'_1 & B'_1 \end{bmatrix} \begin{Bmatrix} a_1 \\ b_1 \end{Bmatrix} = \frac{1}{W_2} \begin{bmatrix} B_2 & -B_2 \\ -A'_2 & A_2 \end{bmatrix} \begin{bmatrix} A_1 & B_1 \\ A'_1 & B'_1 \end{bmatrix} \begin{Bmatrix} a_1 \\ b_1 \end{Bmatrix} \quad (10)$$

Here, A_i and A'_i respectively denote $A(X; k_i)$ and $A_x(X; k_i)$, $i = 1, 2$. Similarly, B_i and B'_i respectively denote $B(X; k_i)$ and $B_x(X; k_i)$, $i = 1, 2$. Also, $W_2 = W(X; k_2)$. Hence, we get

$$\{C_2\} = [Q^{1 \rightarrow 2}] \{C_1\} = \begin{bmatrix} q_{11}^{1 \rightarrow 2} & q_{12}^{1 \rightarrow 2} \\ q_{21}^{1 \rightarrow 2} & q_{22}^{1 \rightarrow 2} \end{bmatrix} \{C_1\} \quad (11)$$

Here, $[Q^{1 \rightarrow 2}]$ is referred to as the jump transfer matrix with the elements

$$\begin{aligned} q_{11}^{1 \rightarrow 2} &= \frac{B'_2 A_1 - B_2 A'_1}{W_2} & q_{12}^{1 \rightarrow 2} &= \frac{B'_2 B_1 - B_2 B'_1}{W_2} \\ q_{21}^{1 \rightarrow 2} &= \frac{A'_1 A_2 - A_1 A'_2}{W_2} & q_{22}^{1 \rightarrow 2} &= \frac{B'_1 A_2 - B_1 A'_2}{W_2} \end{aligned} \quad (12)$$

and

$$\{C_i\} = \left\{ \begin{array}{c} a_i \\ b_i \end{array} \right\}, i = 1, 2 \quad (13)$$

Properties of jump transfer matrices have been extensively discussed in earlier works. But for the sake of convenience we mention a few

$$\begin{aligned} |Q^{1 \rightarrow 2}| &= \frac{W_1}{W_2} \\ [Q^{m \rightarrow n}] &= [Q^{n-1 \rightarrow n}] [Q^{n-2 \rightarrow n-1}] \dots [Q^{m+1 \rightarrow m+2}] [Q^{m \rightarrow m+1}] \\ [Q^{m \rightarrow n}]^{-1} &= [Q^{n \rightarrow m}] \end{aligned} \quad (14)$$

corresponding respectively to the determinant, combination, and inversion properties. Moreover, we readily notice that $|Q^{m \rightarrow n}| = W_m/W_n$. It is clear that a given transfer matrix $[Q^{1 \rightarrow 2}]$ is not invertible unless the Wronskian (4) does not vanish. The combination property explains how to obtain the total transfer matrix over a number of finite jumps, among which the eigenvalue function $k(x)$ is constant.

2.2. Differential Transfer Matrix. Now, we let $k(x)$ be a smooth function of x . Within the infinitesimal neighborhood of any given point such as $x = X$, the eigenvalue function $k(x)$ will undergo a first-order change from $k_1 = k(X)$ to $k_2 = k(X + \Delta x)$. We may then define $k_2 = k_1 + \Delta k$, where Δk represents a small change in the eigenvalue. If Δx is small, then we may neglect the variations of $k(x)$ within $[X, X + \Delta x]$. The corresponding first order change in the vector $\{C\}$ across $x = X$ will be clearly given by

$$\{\Delta C\} \approx \frac{1}{\Delta x} ([Q^{1 \rightarrow 2}] - [I]) \{C_1\} \quad (15)$$

where the approximation becomes exact if we let Δx approach zero. Thereby, we get

$$d\{C(x)\} = [U(x)] \{C(x)\} dx \quad (16)$$

in which $\{C(x)\}$ is the envelope vector function, and the Kernel matrix $[U(x)]$ is

$$[U(x)] = \begin{bmatrix} u_{11}(x) & u_{12}(x) \\ u_{21}(x) & u_{22}(x) \end{bmatrix} = \lim_{\Delta x \rightarrow 0} \frac{1}{\Delta x} ([Q^{1 \rightarrow 2}] - [I]) \quad (17)$$

We notice that in order to obtain the correct solution to the Kernel matrix $[U(x)]$, one needs to make the replacements $G_1 = G$, $G'_1 = G_x$, and $G_2 = G + G_k \Delta k$, $G'_2 = G_x + G_{xk} \Delta k$, where represents either of A or B . Here, subscripts refer to partial derivatives in the sense that $G_x = \partial G / \partial x$, $G_k = \partial G / \partial k$, $G_{xk} = \partial^2 G / \partial x \partial k$. After doing some algebra and simplification we get the complete form for the elements of the Kernel matrix $[U(x)]$ as

$$\begin{aligned} u_{11} &= k' \frac{A_{xk}B - A_kB_x}{W} & u_{12} &= k' \frac{B_{xk}B - B_kB_x}{W} \\ u_{21} &= k' \frac{A_kA_x - A_{xk}A}{W} & u_{22} &= k' \frac{A_xB_k - AB_{xk}}{W} \end{aligned} \quad (18)$$

Here, $k' = \partial k(x) / \partial x$ and $W = AB_x - A_xB$. In the fully expanded form we have

$$\begin{aligned}
u_{11}(x) &= \frac{k'(x)}{W(x)} \left\{ \frac{\partial^2 A[x; k(x)]}{\partial x \partial k} B[x; k(x)] - \frac{\partial A[x; k(x)]}{\partial k} \frac{\partial B[x; k(x)]}{\partial x} \right\} \\
u_{12}(x) &= \frac{k'(x)}{W(x)} \left\{ \frac{\partial^2 B[x; k(x)]}{\partial x \partial k} B[x; k(x)] - \frac{\partial B[x; k(x)]}{\partial k} \frac{\partial B[x; k(x)]}{\partial x} \right\} \\
u_{21}(x) &= \frac{k'(x)}{W(x)} \left\{ \frac{\partial A[x; k(x)]}{\partial k} \frac{\partial A[x; k(x)]}{\partial x} - \frac{\partial^2 A[x; k(x)]}{\partial x \partial k} A[x; k(x)] \right\} \\
u_{22}(x) &= \frac{k'(x)}{W(x)} \left\{ \frac{\partial A[x; k(x)]}{\partial x} \frac{\partial B[x; k(x)]}{\partial k} - A[x; k(x)] \frac{\partial^2 B[x; k(x)]}{\partial x \partial k} \right\}
\end{aligned} \tag{19}$$

where

$$W(x) = A[x; k(x)] \frac{\partial B[x; k(x)]}{\partial x} - \frac{\partial A[x; k(x)]}{\partial x} B[x; k(x)] \tag{20}$$

A general solution to (2) is given by (5) with

$$\{C'(x)\} = [U(x)] \{C(x)\} \tag{21}$$

in which the elements of the Kernel matrix $[U(x)]$ are given in (18). Interestingly, (21) allows an analytical solution through perturbation theory as [2, 6]

$$\begin{aligned}
\{C(x_2)\} &= \{C(x_1)\} + \int_{x_1}^{x_2} [U(y_0)] \{C(y_0)\} dy_0 \\
&+ \int_{x_1}^{x_2} \int_{x_1}^{y_1} [U(y_1)] [U(y_0)] \{C(y_0)\} dy_0 dy_1 \\
&+ \int_{x_1}^{x_2} \int_{x_1}^{y_2} \int_{x_1}^{y_1} [U(y_2)] [U(y_1)] [U(y_0)] \{C(y_0)\} dy_0 dy_1 dy_2 + \dots
\end{aligned} \tag{22}$$

Often (22) is written symbolically as

$$\begin{aligned}
\{C(x_2)\} &= \mathbb{T} \exp \left\{ \int_{x_1}^{x_2} [U(x)] dx \right\} \{C(x_1)\} \\
&= \{C(x_1)\} + \int_{x_1}^{x_2} [U(y_0)] \{C(y_0)\} dy_0 \\
&+ \frac{1}{2!} \int_{x_1}^{x_2} \int_{x_1}^{y_1} \mathbb{T} [U(y_1)] [U(y_0)] \{C(y_0)\} dy_0 dy_1 \\
&+ \frac{1}{3!} \int_{x_1}^{x_2} \int_{x_1}^{y_2} \int_{x_1}^{y_1} \mathbb{T} [U(y_2)] [U(y_1)] [U(y_0)] \{C(y_0)\} dy_0 dy_1 dy_2 + \dots \\
&= [Q^{x_1 \rightarrow x_2}] \{C(x_1)\}
\end{aligned} \tag{23}$$

where $[Q^{x_1 \rightarrow x_2}]$ is the transfer matrix from x_1 to x_2 and $\exp(\cdot)$ being the matrix exponentiation

$$\exp[M] = [I] + \sum_{n=1}^{\infty} \frac{1}{n!} [M]^n \tag{24}$$

Furthermore, \mathbb{T} is the Dyson's ordering operator defined as

$$\mathbb{T} [U(a)] [U(b)] = \begin{cases} [U(a)] [U(b)], & a > b \\ [U(b)] [U(a)], & a < b \end{cases} \tag{25}$$

There are few known sufficient conditions [6, 16], which rarely happen and under which \mathbb{T} may be dropped exactly to reach

$$\{C(x_2)\} = \exp \left\{ \int_{x_1}^{x_2} [U(x)] dx \right\} \{C(x_1)\} \quad (26)$$

The most important sufficient condition includes the case when the Kernel matrix commutes with itself as $[U(a)][U(b)] = [U(b)][U(a)]$ for all given a and b . This is better known as the Lappo-Danilevskii [17] criterion, and is also generalized by Fedorov [18]. Evidently, this condition applies to all constant as well as diagonal Kernel matrices. It is therefore a challenge to find construct the proper extended eigenvalue equation in such a way that the corresponding Kernel matrix meets any of these sufficient criteria. If possible, then exact and explicit closed form solutions to (2) are found analytically by using (26) instead of (23).

While in general, (26) is merely an approximation to the exact solution (23), nevertheless, in any case the determinant and trace of $[Q^{x_1 \rightarrow x_2}]$ would be preserved exactly, meaning that the eigenvalues of the transfer matrix $[Q^{x_1 \rightarrow x_2}]$ would not be affected at least. This allows us to formulate a very convenient approximate numerical solution to the extended problem (2).

2.3. Properties of Differential Transfer Matrix. Properties of the transfer matrix $[Q^{x_1 \rightarrow x_2}]$ as defined in (23) are very much similar to those of the jump transfer matrix (14), given by

$$\begin{aligned} [Q^{x_1 \rightarrow x_1}] &= [I] \\ [Q^{x_1 \rightarrow x_2}] &= \frac{W_1}{W_2} \\ [Q^{x_1 \rightarrow x_2}] &= [Q^{x_3 \rightarrow x_2}] [Q^{x_1 \rightarrow x_3}] \\ [Q^{x_1 \rightarrow x_2}]^{-1} &= [Q^{x_2 \rightarrow x_1}] \end{aligned} \quad (27)$$

Properties of the transfer matrix in which $W_i = W[x_i; k_i] = W[x_i; k(x_i)]$, $i = 1, 2$. The first property, the identity property readily follows by definition in (23). The determinant property can be observed by noting that Dyson's operator has no effect on the determinant, and thus

$$\begin{aligned} |Q^{x_1 \rightarrow x_2}| &= \left| \mathbb{T} \exp \left\{ \int_{x_1}^{x_2} [U(x)] dx \right\} \right| = \left| \exp \left\{ \int_{x_1}^{x_2} [U(x)] dx \right\} \right| \\ &= \exp \left(\text{tr} \left\{ \int_{x_1}^{x_2} [U(x)] dx \right\} \right) = \exp \left(\int_{x_1}^{x_2} [u_{11}(x) + u_{22}(x)] dx \right) \end{aligned} \quad (28)$$

Now from (18) we get

$$\begin{aligned} \int_{x_1}^{x_2} [u_{11}(x) + u_{22}(x)] dx &= \int_{x_1}^{x_2} \frac{A_{xk}B - AB_{xk}}{AB_x - BA_x} k' dx = - \int_{x_1}^{x_2} \frac{\partial}{\partial k} \ln W \frac{\partial k}{\partial x} dx \\ &= - \int_{k_1}^{k_2} \frac{\partial}{\partial k} \ln W dk = \ln k_1 - \ln k_2 \end{aligned} \quad (29)$$

Inserting this result in (28) gives the determinant property in (28). Combination and inversion properties also follow the definition (23).

2.4. Fundamental Theorem. In this section, we rigorously show that the differential transfer matrix method leads to an exact solution of the differential equation (2). To show this, we start by proving the so-called *Derivative Lemma*.

Lemma 2.4.1. *The total derivative of function (5) is given by*

$$\frac{d^n}{dx^n} f[x; k(x)] = a(x) \frac{\partial^n}{\partial x^n} A[x; k(x)] + b(x) \frac{\partial^n}{\partial x^n} B[x; k(x)], \quad 0 \leq n \leq 2 \quad (30)$$

Proof. Proof follows by direct substitution. The case of $n = 0$ is trivial, and we first prove the validity of (30) for $n = 1$. Direct differentiation of (5) by chain rule gives

$$\frac{d}{dx} f = a' A + b' B + a(A_x + k' A_k) + b(B_x + k' B_k) \quad (31)$$

where $f = aA + bB$. But we already have obtained the derivatives a' and b' from (21) and (18) as

$$\begin{aligned} a' &= u_{11}a + u_{12}b = \frac{k'}{W} [(A_{xk}B - A_kB_x)a + (B_{xk}B - B_kB_x)b] \\ b' &= u_{21}a + u_{22}b = \frac{k'}{W} [(A_kA_x - A_{xk}A)a + (B_kA_x - B_{xk}A)b] \end{aligned} \quad (32)$$

in which the elements $u_{ij}, i, j = 1, 2$ of the Kernel matrix are given in (18). After some minor algebra we get

$$\frac{d}{dx} f = aA_x + bB_x \quad (33)$$

To show the correctness of (30) for $n = 2$, we take the derivative again with respect to x from both sides of (30), thus giving

$$\begin{aligned} \frac{d^2}{dx^2} f &= \frac{d}{dx} (aA_x + bB_x) \\ &= a'A_x + b'B_x + a\frac{d}{dx} A_x + b\frac{d}{dx} B_x \\ &= (u_{11}a + u_{12}b)A_x + (u_{21}a + u_{22}b)B_x \\ &\quad + a(A_{xx} + k'A_{xk}) + b(B_{xx} + k'B_{xk}) \end{aligned} \quad (34)$$

Further substitution of (32) in (34) gives

$$\begin{aligned} \frac{d^2}{dx^2} f &= \frac{k'}{AB_x - BA_x} [(A_{xk}B - A_kB_x)a + (B_{xk}B - B_kB_x)b] A_x \\ &\quad + \frac{k'}{AB_x - BA_x} [(A_kA_x - A_{xk}A)a + (B_kA_x - B_{xk}A)b] B_x \\ &\quad + a(A_{xx} + k'A_{xk}) + b(B_{xx} + k'B_{xk}) \end{aligned} \quad (35)$$

Here, we have used the definition of the Wronskian $W = AB_x - BA_x$ from (4). Eventually, after some algebra we arrive at the final result

$$\frac{d^2}{dx^2} f = aA_{xx} + bB_{xx} \quad (36)$$

This completes the proof □

We are now in a position to present the *Fundamental Theorem of Differential Transfer Matrix Method* as follows.

Theorem 2.4.2. *The solution to (2) having the form (5) with (21) is exact.*

Proof. To show the validity of the statement, we start by plugging in (5) directly into (2).

$$\begin{aligned}\mathbb{L}_k f[x; k] &= \mathbb{L}_k \{aA[x; k] + bB[x; k]\} \\ &= a\mathbb{H}_k A[x; k] + b\mathbb{H}_k B[x; k]\end{aligned}\quad (37)$$

where \mathbb{H}_k and \mathbb{L}_k are respectively defined in (1) and (2). Here, the explicit dependence of the operator \mathbb{L}_k and functions a , b , and k on x is not shown. But by assumption we have $\mathbb{H}_k A[x; k] = \mathbb{H}_k B[x; k] = 0$ and hence the assertion. \square

All remains is to force the initial or boundary conditions, and we here mention the treatment of both types of conditions.

2.5. Initial Conditions. Without loss of generality, we may assume that initial conditions are known at some point like $x = c$. Suppose that $f(c)$ and $f'(c)$ are known. Then by derivative lemma (30) we have

$$f'(x) = A_x[x; k(x)]a(x) + B_x[x; k(x)]b(x) \quad (38)$$

Therefore we get

$$\begin{Bmatrix} f(c) \\ f'(c) \end{Bmatrix} = \begin{bmatrix} A[c; k(c)] & B[c; k(c)] \\ A_x[c; k(c)] & B_x[c; k(c)] \end{bmatrix} \begin{Bmatrix} a(c) \\ b(c) \end{Bmatrix} \quad (39)$$

Thus we may obtain the initial vector $\{C(c)\}$ as

$$\{C(c)\} = \begin{bmatrix} A[c; k(c)] & B[c; k(c)] \\ A_x[c; k(c)] & B_x[c; k(c)] \end{bmatrix}^{-1} \begin{Bmatrix} f(c) \\ f'(c) \end{Bmatrix} \quad (40)$$

with the solution

$$\{C(c)\} = \frac{1}{W[c; k(c)]} \begin{bmatrix} B_x[c; k(c)] & -B[c; k(c)] \\ -A_x[c; k(c)] & A[c; k(c)] \end{bmatrix} \begin{Bmatrix} f(c) \\ f'(c) \end{Bmatrix} \quad (41)$$

Now by (23) we have the full solution to the envelope vector as

$$\begin{aligned}\{C(x)\} &= \mathbb{T} \exp \left\{ \int_c^x [U(y)] dy \right\} \{C(c)\} \\ &\approx \exp \left\{ \int_c^x [U(y)] dy \right\} \{C(c)\}\end{aligned}\quad (42)$$

This allows us to obtain the final solution to the initial value problem (2) as

$$f(x) = \begin{bmatrix} A[x; k(x)] & B[x; k(x)] \end{bmatrix} \{C(x)\} \quad (43)$$

2.6. Boundary Conditions. Without loss of generality, we may assume that boundary conditions are known at two points like $x = c_1, c_2$. Suppose that $f(c_1)$ and $f(c_2)$ are known. Then by (5) we have

$$\begin{aligned}f(c_1) &= \begin{bmatrix} A[c_1; k(c_1)] & B[c_1; k(c_1)] \end{bmatrix} \{C(c_1)\} \\ f(c_2) &= \begin{bmatrix} A[c_2; k(c_2)] & B[c_2; k(c_2)] \end{bmatrix} \{C(c_2)\}\end{aligned}\quad (44)$$

But from (23) we have

$$\{C(c_2)\} = [Q^{c_1 \rightarrow c_2}] \{C(c_1)\} \quad (45)$$

Thus by combining (44) and (45) we may obtain the system of equations

$$\begin{Bmatrix} f(c_1) \\ f(c_2) \end{Bmatrix} = \begin{bmatrix} A[c_1; k(c_1)] & B[c_1; k(c_1)] \\ q_{11}A[c_2; k(c_2)] + q_{21}B[c_2; k(c_2)] & q_{12}A[c_2; k(c_2)] + q_{22}B[c_2; k(c_2)] \end{bmatrix} \begin{Bmatrix} C(c_1) \end{Bmatrix} \quad (46)$$

with the solution

$$\begin{aligned} \{C(c_1)\} &= \begin{bmatrix} A[c_1; k(c_1)] & B[c_1; k(c_1)] \\ q_{11}A[c_2; k(c_2)] + q_{21}B[c_2; k(c_2)] & q_{12}A[c_2; k(c_2)] + q_{22}B[c_2; k(c_2)] \end{bmatrix}^{-1} \times \\ &\quad \begin{Bmatrix} f(c_1) \\ f(c_2) \end{Bmatrix} \\ \{C(c_2)\} &= [Q^{c_1 \rightarrow c_2}] \{C(c_1)\} \end{aligned} \quad (47)$$

The rest is the same and similar to (42)

$$\begin{aligned} \{C(x)\} &= \mathbb{T} \exp \left\{ \int_{c_1}^x [U(y)] dy \right\} \{C(c_1)\} = \mathbb{T} \exp \left\{ - \int_x^{c_2} [U(y)] dy \right\} \{C(c_2)\} \\ &\approx \exp \left\{ \int_{c_1}^x [U(y)] dy \right\} \{C(c_1)\} \approx \exp \left\{ - \int_x^{c_2} [U(y)] dy \right\} \{C(c_2)\} \end{aligned} \quad (48)$$

3. EXAMPLES

In this section, we present some application examples describing the details of the method.

3.1. Wave Equation. Numerous physical problems are described via the simple second-order equation

$$\psi''(x) + k^2(x) \psi(x) = 0 \quad (49)$$

The equation (49) is known to have no explicit solution for arbitrary eigenvalue function $k(x)$, which in the literature is usually referred to as the wavenumber function. The only existing analytical solution to (49) is the very well-known WKB approximation. Here, the corresponding operators read

$$\mathbb{H}_k = \frac{\partial^2}{\partial x^2} + k^2 \quad \mathbb{L}_{k(x)} = \frac{d^2}{dx^2} + k^2(x) \quad (50)$$

In case of constant wavenumber, any solution of (49) is given by linear combinations of exponential functions $\exp(\pm ikx)$, and therefore the eigenfunctions are readily found to be

$$A[x; k(x)] = \exp[-ikx(x)] \quad B[x; k(x)] = \exp[+ikx(x)] \quad (51)$$

with the Wronskian $W[x; k(x)] = 2ik(x)$. To find a solution to (49) it is therefore sufficient to find the Kernel matrix $[U(x)]$, which is

$$[U(x)] = \frac{k'(x)}{2k(x)} \begin{bmatrix} -1 + 2ixk(x) & \exp[+2ixk(x)] \\ \exp[-2ixk(x)] & -1 - 2ixk(x) \end{bmatrix} \quad (52)$$

Numerical and analytical solutions of (49) using the Kernel matrix (52) has been extensively studied in the literature through past years.

3.2. Airy's Equation. One of the known problems with the above differential transfer matrix solution of (49) is occurrence of singularities at which $k^2(x)$ changes sign and the Wronskian vanishes, better known as returning points. The singularity is clear in (52) as the denominator. Even the approximate WKB solution fails near returning points. It is a common practice however to expand the solution near the returning points via Airy functions. Without loss of generality we may assume that the singularity is located at $x = 0$. In this case, we present a slightly modified form of (49) as

$$\psi''(x) - k^3(x)x\psi(x) = 0 \quad (53)$$

with the Airy wavenumber satisfying $k(0) \neq 0$. Hence,

$$\mathbb{H}_k = \frac{\partial^2}{\partial x^2} - k^3 x \quad \mathbb{L}_{k(x)} = \frac{d^2}{dx^2} - k^3(x)x \quad (54)$$

In case of constant wavenumber, any solution of (53) is given by linear combinations of Airy functions $\text{Ai}(kx)$ and $\text{Bi}(kx)$, and thus the eigenfunctions take the form

$$A[x; k(x)] = \text{Ai}[xk(x)] \quad B[x; k(x)] = \text{Bi}[xk(x)] \quad (55)$$

having the constant Wronskian $W[x; k(x)] = 1/\pi$. This choice of basis, after some simplification, leads to the following Kernel matrix elements

$$\begin{aligned} u_{11} &= +\pi k' \{k^2 x^2 \text{Ai}(kx) \text{Bi}(kx) + \text{Ai}'(kx) [\text{Bi}(kx) - kx \text{Bi}'(kx)]\} \\ u_{12} &= \pi k' \{ \text{Bi}'(kx) [\text{Bi}(kx) - kx \text{Bi}'(kx)] + k^2 x^2 \text{Bi}^2(kx) \} \\ u_{21} &= \pi k' \{ \text{Ai}'(kx) [xk \text{Ai}'(kx) - \text{Ai}(kx)] - k^2 x^2 \text{Ai}^2(kx) \} \\ u_{22} &= -\pi k' \{ k^2 x^2 \text{Ai}(kx) \text{Bi}(kx) + \text{Bi}'(kx) [\text{Ai}(kx) - kx \text{Ai}'(kx)] \} \end{aligned} \quad (56)$$

which is clearly non-singular at $x = 0$. Here, dependence of the eigenvalue function $k(x)$ on x is not displayed for the sake of convenience.

3.3. Bessel's Equation. In the domain of fiber optics having cylindrical symmetry and after proper transformations, the radial component of the wave equation takes the form

$$x^2 \psi''(x) + x \psi'(x) + [k^2(x)x^2 - \nu^2] \psi(x) = 0 \quad (57)$$

Hence

$$\mathbb{H}_k = x^2 \frac{\partial^2}{\partial x^2} + x \frac{\partial}{\partial x} + (k^2 x^2 - \nu^2) \quad \mathbb{L}_{k(x)} = x^2 \frac{d^2}{dx^2} + x \frac{d}{dx} + [k^2(x)x^2 - \nu^2] \quad (58)$$

In case of constant wavenumber, any solution of (57) is given by any linear combinations of Bessel and Neumann functions $J_\nu(kx)$ and $N_\nu(kx)$, or Hankel functions $H_\nu^{(1)}(kx)$ and $H_\nu^{(2)}(kx)$. For the first pair the eigenfunctions take the form

$$A[x; k(x)] = J_\nu[xk(x)] \quad B[x; k(x)] = N_\nu[xk(x)] \quad (59)$$

having the Wronskian $W[x; k(x)] = 2/\pi x$. The elements of the corresponding Kernel matrix are

$$\begin{aligned} u_{11} &= +\frac{x\pi k'}{2} \{ [kx [J_{\nu-2}(kx) - 2J_\nu(kx) + J_{\nu+2}(kx)] + 2[J_{\nu-1}(kx) - J_{\nu+1}(kx)] N_\nu(kx) \\ &\quad - kx [J_{\nu-1}(kx) - J_{\nu+1}(kx)] [N_{\nu-1}(kx) - N_{\nu+1}(kx)] \} \\ u_{12} &= -\frac{x\pi k'}{2} \{ [kx [N_{\nu-2}(kx) - 2N_\nu(kx) + N_{\nu+2}(kx)] + 2[N_{\nu-1}(kx) - N_{\nu+1}(kx)] N_\nu(kx) \\ &\quad + kx [N_{\nu-1}(kx) - N_{\nu+1}(kx)]^2 \} \\ u_{21} &= +\frac{x\pi k'}{2} \{ [kx [J_{\nu-2}(kx) - 2J_\nu(kx) + J_{\nu+2}(kx)] + 2[J_{\nu-1}(kx) - J_{\nu+1}(kx)] J_\nu(kx) \\ &\quad + kx [J_{\nu-1}(kx) - J_{\nu+1}(kx)]^2 \} \\ u_{22} &= -\frac{x\pi k'}{2} \{ [kx [N_{\nu-2}(kx) - 2N_\nu(kx) + N_{\nu+2}(kx)] + 2[N_{\nu-1}(kx) - N_{\nu+1}(kx)] J_\nu(kx) \\ &\quad - kx [J_{\nu-1}(kx) - J_{\nu+1}(kx)] [N_{\nu-1}(kx) - N_{\nu+1}(kx)] \} \end{aligned} \quad (60)$$

As it can be seen, all elements of the Kernel matrix vanish at $x = 0$; this ensures cylindrical symmetry of the radial function.

It should be also noticed that since Bessel functions with non-integer order are well-defined [19]

$$J_\alpha(x) = \sum_{m=0}^{\infty} \frac{(-1)^m}{m! \Gamma(m + \alpha + 1)} \left(\frac{x}{2}\right)^{2m+\alpha} \quad (61)$$

One could have also replaced the eigenvalue function with the order as

$$x^2 \psi''(x) + x \psi'(x) + [x^2 - k^2(x)] \psi(x) = 0 \quad (62)$$

Hence

$$\mathbb{H}_k = x^2 \frac{\partial^2}{\partial x^2} + x \frac{\partial}{\partial x} + (x^2 - k^2) \quad \mathbb{L}_{k(x)} = x^2 \frac{d^2}{dx^2} + x \frac{d}{dx} + [x^2 - k^2(x)] \quad (63)$$

Again since $J_\alpha(x)$ and $J_{-\alpha}(x)$ for non-integer α are linearly independent, the natural choice of eigenfunctions based on Bessel functions would be either

$$A[x; k(x)] = J_{+k(x)}(x) \quad B[x; k(x)] = J_{-k(x)}(x) \quad (64)$$

or

$$A[x; k(x)] = J_{k(x)}(x) \quad B[x; k(x)] = N_{k(x)}(x) \quad (65)$$

The latter pair has the same Wronskian of $W[x; k(x)] = 2/\pi x$. Hence, the elements of the Kernel matrix are

$$\begin{aligned} u_{11}(x) &= \frac{\pi x k'(x)}{2} \left\{ \frac{\partial^2 J_{k(x)}(x)}{\partial x \partial k} N_{k(x)}(x) - \frac{\partial J_{k(x)}(x)}{\partial k} \frac{\partial N_{k(x)}(x)}{\partial x} \right\} \\ u_{12}(x) &= \frac{\pi x k'(x)}{2} \left\{ \frac{\partial^2 N_{k(x)}(x)}{\partial x \partial k} N_{k(x)}(x) - \frac{\partial N_{k(x)}(x)}{\partial k} \frac{\partial N_{k(x)}(x)}{\partial x} \right\} \\ u_{21}(x) &= \frac{\pi x k'(x)}{2} \left\{ \frac{\partial J_{k(x)}(x)}{\partial k} \frac{\partial J_{k(x)}(x)}{\partial x} - \frac{\partial^2 J_{k(x)}(x)}{\partial x \partial k} J_{k(x)}(x) \right\} \\ u_{22}(x) &= \frac{\pi x k'(x)}{2} \left\{ \frac{\partial J_{k(x)}(x)}{\partial x} \frac{\partial N_{k(x)}(x)}{\partial k} - J_{k(x)}(x) \frac{\partial^2 N_{k(x)}(x)}{\partial x \partial k} \right\} \end{aligned} \quad (66)$$

3.4. Euler-Cauchy Equation. The Euler-Cauchy equation reads

$$x^2 \psi''(x) + x \psi'(x) - k^2(x) \psi(x) = 0 \quad (67)$$

Therefore, the corresponding operators are given by

$$\mathbb{H}_k = x^2 \frac{\partial^2}{\partial x^2} + x \frac{\partial}{\partial x} - k^2 \quad \mathbb{L}_{k(x)} = x^2 \frac{d^2}{dx^2} + x \frac{d}{dx} - k^2(x) \quad (68)$$

When $k(x)$ is a constant, solutions of (67) are given by linear combinations of x^{+k} and x^{-k} . Thus, the extended basis functions are

$$A[x; k(x)] = x^{+k(x)} \quad B[x; k(x)] = x^{-k(x)} \quad (69)$$

with the Wronskian $W[x; k(x)] = -2k(x)/x$, which vanishes at $k(x) = 0$. The Kernel matrix simplifies to the convenient form

$$[U(x)] = -\frac{k'(x)}{2k(x)} \begin{bmatrix} 1 + 2k(x) \ln x & -x^{-2k(x)} \\ -x^{2k(x)} & 1 - 2k(x) \ln x \end{bmatrix} \quad (70)$$

3.5. Approximate Solution. The exact matrix exponential in (23) can be evaluated if off-diagonal elements of the Kernel matrix could be dropped. This has been previously shown to lead to the well-known WKB solution [4, 7, 8]. Under such conditions, the approximate differential transfer matrix takes the form

$$\begin{aligned} [Q^{x_1 \rightarrow x_2}] &= \mathbb{T} \exp \left\{ \int_{x_1}^{x_2} [U(x)] dx \right\} \approx \mathbb{T} \exp \left\{ \int_{x_1}^{x_2} \begin{bmatrix} u_{11}(x) & 0 \\ 0 & u_{22}(x) \end{bmatrix} dx \right\} \\ &= \begin{bmatrix} \exp \left[\int_{x_1}^{x_2} u_{11}(x) dx \right] & 0 \\ 0 & \exp \left[\int_{x_1}^{x_2} u_{22}(x) dx \right] \end{bmatrix} \end{aligned} \quad (71)$$

3.6. Periodic Perturbations. There is a great deal of simplification possible, when the eigenvalue function $k(x) = k(x+L)$ is periodic for some $L > 0$. Let \mathbb{T}_L be the translation operator, defined as $\mathbb{T}_L h(x) = h(x+L)$, for all arbitrary functions $h(x)$. Hence, we readily have the commutation property $[\mathbb{L}_{k(x)}, \mathbb{T}_L] = 0$, and hence these two operators share identical eigenfunctions. Since $\mathbb{L}_{k(x)}$ is supposed to be linear, Bloch-Floquet theorem [9] applies and then any solution will take the form of Bloch eigenfunctions

$$\mathbb{T}_L f[x; k(x)] = f[x+L; k(x+L)] = \exp(-j\kappa L) f[x; k(x)] \quad (72)$$

in which the complex number κ is being referred to as the Bloch number. This shows that $f[x; k(x)]$ is an eigenfunction of the translation operator \mathbb{T}_L with the eigenvalue $\exp(-j\kappa L)$. Based on (72), we furthermore have

$$f(x) = \exp(-j\kappa x) g_\kappa(x) \quad (73)$$

with the envelope function satisfying

$$\mathbb{T}_L g_\kappa(x) = g_\kappa(x) \quad (74)$$

Under such circumstances, it is easy to obtain the characteristic equation of eigenfunctions. From (5) and (72) we have

$$\begin{aligned}\mathbb{T}_L f[x; k(x)] &= a(x+L) A[x+L; k(x)] + b(x+L) B[x+L; k(x)] \\ &= \exp(-j\kappa L) \{a(x) A[x; k(x)] + b(x) B[x; k(x)]\}\end{aligned}\quad (75)$$

By taking differentiating with respect to x from (72) and derivative lemma (30) we also get

$$\begin{aligned}\mathbb{T}_L f'[x; k(x)] &= \exp(-j\kappa L) f'[x; k(x)] \\ &= \exp(-j\kappa L) \{a(x) A_x[x; k(x)] + b(x) B_x[x; k(x)]\}\end{aligned}\quad (76)$$

We furthermore notice that (75) and (76) are actually identities which hold for all x . These two can be combined to get the system of equations

$$\begin{aligned}\begin{bmatrix} A[x+L; k(x)] & B[x+L; k(x)] \\ A_x[x+L; k(x)] & B_x[x+L; k(x)] \end{bmatrix} \{C(x+L)\} &= \\ \exp(-j\kappa L) \begin{bmatrix} A[x; k(x)] & B[x; k(x)] \\ A_x[x; k(x)] & B_x[x; k(x)] \end{bmatrix} \{C(x)\} &\end{aligned}\quad (77)$$

which allows the solution

$$\begin{aligned}\mathbb{T}_L \{C(x)\} &= \frac{\exp(-j\kappa L)}{W[x+L; k(x)]} \begin{bmatrix} B_x[x+L; k(x)] & -B[x+L; k(x)] \\ -A_x[x+L; k(x)] & A[x+L; k(x)] \end{bmatrix} \times \\ &\quad \begin{bmatrix} A[x; k(x)] & B[x; k(x)] \\ A_x[x; k(x)] & B_x[x; k(x)] \end{bmatrix} \{C(x)\} \\ &= \exp(-j\kappa L) [V] \{C(x)\}\end{aligned}\quad (78)$$

But from (26)

$$\mathbb{T}_L \{C(x)\} = [Q^{x \rightarrow x+L}] \{C(x)\} \quad (79)$$

Simultaneous satisfaction of (77) and (78) requires that

$$|\exp(-j\kappa L) [V] - [Q]| = 0 \quad (80)$$

In other words, we should have

$$\kappa = \frac{j}{L} \ln \{\text{eig}[P]\} \quad (81)$$

in which $[P] = [V]^{-1} [Q]$. Here, constancy of the Bloch wavenumber κ is guaranteed by Bloch-Floquet theorem, and is rigorously shown to hold for the example of extended wave equation (49) with periodic wavenumber in [9].

4. CONCLUSIONS

In this paper, we presented a new analytical solution obtained by differential transfer matrix method to a wide class of second-order linear differential equations, which are extended from eigenvalue problems by replacing the eigenvalue with an arbitrary eigenvalue function. We presented the details of the method and a fundamental theorem to rigorously establish the mathematical formulation. Few examples were also described.

REFERENCES

- [1] M. Razavy, *Quantum Theory of Tunneling*, World Scientific, 2003.
- [2] W. Schleich, *Quantum Optics in Phase Space*, Wiley, 2001.
- [3] X.-F. Li, Approximate solution of linear ordinary differential equations with variable coefficients, *Mathematics and Computers in Simulation* 75 (2007) pp. 113125.
- [4] P. Boonserm, M. Visser, Reformulating the Schrödinger equation as a ShabatZakharov system, *Journal of Mathematical Physics* 51 (2010) 022105.
- [5] A. D. Polyanin and V. F. Zaitsev, *Handbook of Exact Solutions for Ordinary Differential Equations*, 2nd Edition, Chapman & Hall/CRC Press, Boca Raton, 2003.
- [6] S. Khorasani, and A. Adibi, Analytical Solution of Linear Ordinary Differential Equations by Differential Transfer Matrix Method, *Electronic Journal of Differential Equations* 2003 (79) (2003), pp. 1-18.
- [7] S. Khorasani and K. Mehrany, Analytical solution of wave equation for arbitrary non-homogeneous media, *Proceedings of SPIE* 4772 (2002), pp. 25-36.
- [8] S. Khorasani and K. Mehrany, Differential transfer matrix method for solution of one-dimensional linear non-homogeneous optical structures, *Journal of Optical Society of America B* 20 (2003), pp. 91-96.
- [9] S. Khorasani, and A. Adibi, New Analytical Approach for Computation of Band Structure in One-dimensional Periodic Media, *Optics Communications* 216 (4-6) (2003) pp. 439-451.
- [10] P. Yeh, *Optical Waves in Layered Media*, Wiley, New York, 1988.
- [11] A. Fassler and E. Stiefel, *Group Theoretical Methods and Their Applications*, Birkhauser, Boston, 1992.
- [12] M. H. Eghlidi, K. Mehrany, and B. Rashidian, Modified differential transfer matrix method for solution of one dimensional linear inhomogeneous optical structures, *Journal of Optical Society of America B* 22 (2005) pp. 1521-1528.
- [13] M .H. Eghlidi, K. Mehrany, and B. Rashidian, Improved differential transfer matrix method for inhomogeneous one-dimensional photonic crystals, *Journal of Optical Society of America B* 23 (2006), pp. 1451-1459.
- [14] N. Zariean, P. Sarrafi, K. Mehrany, and B. Rashidian, Differential-Transfer-Matrix Based on Airy's Functions in Analysis of Planar Optical Structures With Arbitrary Index Profiles, *IEEE Journal of Quantum Electronics* 44 (2008) pp. 324-330.
- [15] M. H. Eghlidi, K. Mehrany, and B. Rashidian, General solution of linear differential equations by using differential transfer matrix method, *Proceedings of the 2005 European Conference on Circuit Theory and Design* 3 (2005), pp. III/113-III/116.
- [16] S. Khorasani, Reply to 'Comment on "Analytical solution of non-homogeneous anisotropic wave equation based on differential transfer matrices"', *Journal of Optics A: Pure and Applied Optics* 5 (2003), pp. 434-435.
- [17] S. A. Mazanik, Linear Differential Lappo-Danilevskii Systems, *Mathematica Bohemica* 127 (2) (2001) pp. 275-282.
- [18] F. I. Fedorov, A generalization of the Lappo-Danilevskii criterion, *Dokl. Akad. Nauk. BSST* 4 (11) (1960) pp. 454-455.
- [19] M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions*, Dover, New York, 1965.

SCHOOL OF ELECTRICAL ENGINEERING, SHARIF UNIVERSITY OF TECHNOLOGY
E-mail address: khorasani@sina.sharif.edu